Acquisition of X-ray Diffractometer

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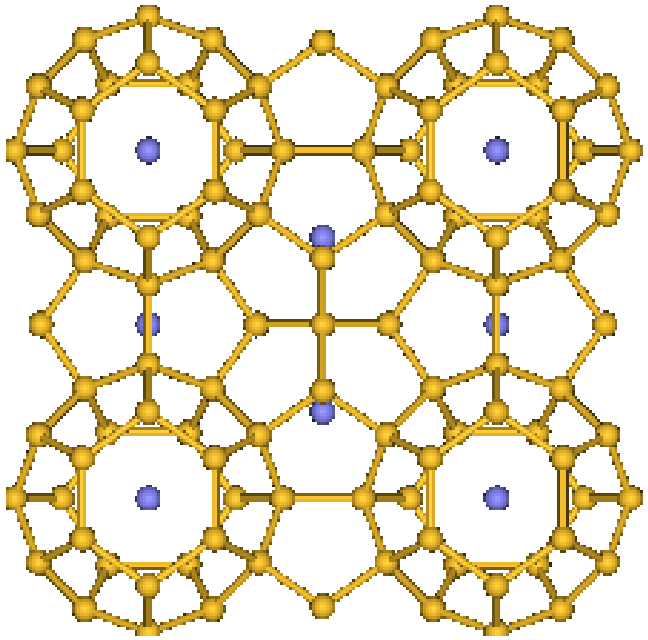
MRI 0216111



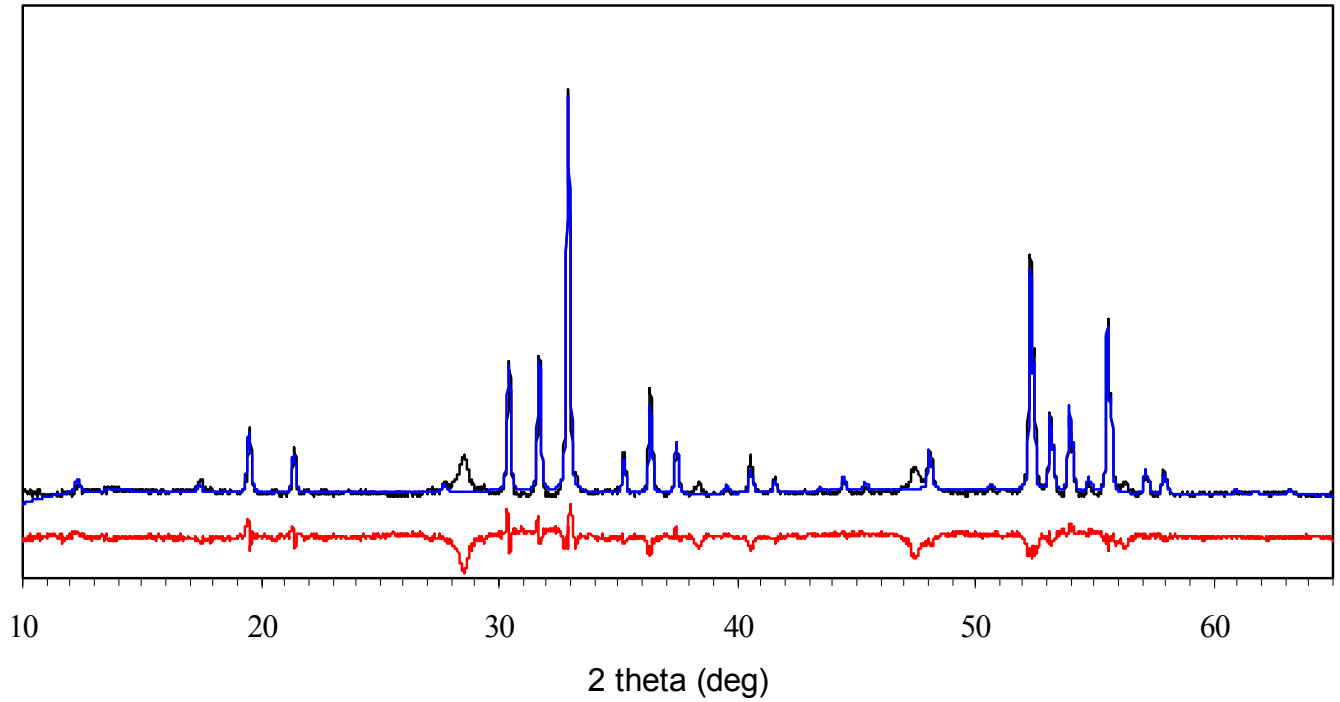
Crystal structure of Na_8Si_{46} clathrate.

A new way of obtaining of group IV clathrates was discovered. We have found that type I clathrate Na_8Si_{46} can be synthesized in a chemical reaction:

$$NaSi + NH_4Br \rightarrow Na_8Si_{46} + NaBr + NH_3 + H_2$$

The yield is approximately 60 %, with main by-product being a microcrystalline silicon. This reaction opens an exciting possibility of synthesis of open framework materials with transition metals encapsulated inside silicon or germanium cages.

The synthesis of type I clathrate was verified with MMA desktop X-ray diffractometer:



The X-ray spectrum of Na_8Si_{46} clathrate synthesized in the reaction of NaSi and NH_4Br. Difference between experimental (black) and fitted (blue) spectra is shown as a read line at the bottom. Two broad peaks (at appox. 28.5^o and 47.5^o) are due to a microcystalline silicon by-product.